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TRACE INORGANIC ELEMENT AND PARTICULATE DEPOSITION MODEL - PART II

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ABSTRACT

This is the second of two reports exploring the dispersion and deposition of trace inorganic elements and particles emitted from coal-fired power plants. The various aspects of trace element transformation, transport and dispersion are examined. A set of criteria for selection of a trace element dispersion and deposition model, suitable for application within Ontario Hydro, is presented. The selection criteria are as follows: (1) The model should be a Gaussian climatological model containing state-of-the-art modules for plume rise, wind shear, reflection, dispersion coefficients, gravitational sedimentation, wet and dry deposition, and particle size distribution; (2) The modelling region of interest should be within a radius of 25 km of the source; (3) The model should be capable of computing seasonal or longer time averages; (4) The model should be tunable for surface characteristics surrounding the Nanticoke, Lakeview, Lambton, Atikokan and Thunder Bay power plants; (5) The model must be implementable on an Ontario Hydro computer, and (6) The model should use a practical amount of computer time and the software should be user friendly.

The next phase of this work will involve the assessment of available models against these modelling criteria and selection of the model to be implemented.

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1.0 INTRODUCTION

Part I of this two-report package dealt with the nature of trace inorganic element and particle releases from coal-fired generating stations, Kalvins (1983). The report identified the chemical and physical forms of trace inorganic emissions. Also addressed in Part I were wet and dry removal processes. To complete the survey, this report will examine trace element in-plume transformations, transport and dispersion processes. The scope of the work is to develop criteria by which a model can be selected. Much of the information for this report was obtained from the Canadian Electrical Asociation (CEA) Project G 194 draft report prepared by Battelle Pacific Northwest Laboratories, Van Voris et al (1984). The CEA report, along with its Phase I counterpart, Evans et al (1984), represent a thorough up-to-date evaluation of the subject. Of course, it is recognized that significant knowledge gaps exist about the atmospheric pathways of trace element emissions.

This report is arranged into sections entitled In-plume Transformation, Transport and Dispersion Processes and Model Selection Criteria. Important points are summarized in the conclusions. Recommendations are offered to complete the report.

2.0 IN PLUME TRANSFORMATIONS

Gaseous and particulate trace inorganics released from the stack undergo transformations as the power plant plume interacts with ambient air. The primary transformation mechanisms are: thermal coagulation (a process involving the capture of submicron particles by larger particles), gravitational sedimentation, adsorption (the process of trace gas deposition to particle surfaces), gas to particle conversions (eg, $SO_2 \rightarrow$ sulfate) and gas reactions. For descriptions of these processes the reader is referred to Sheih (1977), Strauss (1975), Evans et al (1982) and Hobbs et al (1983). The mechanisms by which these transformations proceed and interact with each other within a power plant plume are not well understood. As a result, the only process that is usually addressed when modelling trace elements is gravitational sedimentation. The other processes are treated implicitly by the provision of particle size distribution and trace gas speciation algorithms. This approach is usually justified on the assumption that the in-plume transformations of trace elements are too slow, at typical plume temperatures, to significantly change the release particle size distribution and gas speciation. Additionally, any significant time varying effect of these transformations is further smoothed out by the long time averages considered when modelling trace element deposition.

In summary, it is important when selecting a model to consider what in-plume transformation processes are important for the power plant being modelled. It is recommended that only gravitational sedimentation, particle size distribution and gas speciation modules be considered.

3.0 TRANSPORT AND DISPERSION PROCESSES

Regulatory requirements (ie, present and forecast) influence the selection of transport and dispersion models, as do criteria prescribed by Central Thermal Services Environmental Protection Department personnel. The zone of impact for trace element emissions is within a 25-km radius of the power plant and the time averages are seasonal at a minimum, with annual and longer time averages of more interest. However, if it is feasible Environmental Protection Department would like a model to cover a region of 50 km and episodic analysis as well. Further, model selection is limited by the available meteorological data. Typically the available meteorological data are from class one weather stations, which provide hourly observations of wind speed, wind direction, temperature, precipitation and derived frequencies of parameters such as stability, precipitation, wind speed and wind direction.

These constraints alone limit the number of models that would be appropriate for application. Practical constraints further narrow the range of models. The model must be implementable on an Ontario Hydro computer. The model will be a hybrid of off the shelf models. The model must not require a large amount of computer time to run and the software should be user friendly.

The model must also be tunable to reflect the special terrain features of Hydro's Nanticoke, Lakeview, Lambton, Atikokan and Thunder Bay Thermal Generating Stations.

The above constraints preclude the selection of mathematically sophisticated models. For example, numerical transport and dispersion models require more development time than is desirable and require more input data than are available. Similarly, the selection of statistical transport and diffusion models is not practical at this time because no emissions/monitoring data base for trace elements is available on which to predicate a statistical model.

The remaining group of transport and diffusion models are termed kinematic models. Kinematic refers to the process of simplifying the equations governing pollutant transport and dispersion such that closed analytic solution is achieved. The most common kinematic models obtained closure by specifying a Gaussian concentration distribution. The Gaussian equation is as follows:

$$x(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(\frac{-(y - y_o)^2}{2\sigma_y^2}\right)\left[\exp\left(\frac{-(H - Z_o)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(H + Z_o)^2}{2\sigma_z^2}\right) + R\,(Hm)\right], \quad (1)$$

where:

x = coordinate of the receptor location parallel to the wind direction;

y = coordinate of the receptor location normal to the wind direction;

z = vertical coordinate;

$x_o = 0$, y_o, z_o = coordinate of the emissions source;

Q = continuous emission rate;

H = height of the plume;

u = average wind speed;

$\sigma_y = \sigma_y(x)$ = horizontal dispersion coefficient;

$\sigma_z = \sigma_z(x)$ = vertical dispersion coefficient; and

$R(Hm)$ = reflection terms describing plume reflection at the ground boundary and/or an inversion layer aloft at height Hm.

Assumptions Inherent in Gaussian Models. The basic assumptions inherent in the Gaussian plume model as originally developed are as follows:

- Continuous, non-heated emissions from a near-surface, point source.
- No loss of plume material from chemical or physical removal processes (perfect reflection of the plume).
- Steady-state, uniform atmosphere (not changing in time or space):

  --Straight line flow along mean wind direction.

  --Average wind speed, u, representative of the entire mixed layer.

  --Horizontal and vertical dispersion rates varying only as a function of stability and downwind distances (x).

  -- Time averaged concentrations, x(x,y,z), characteristic of the sampling time of the empirical dispersion coefficients, σ_y and σ_z.

Typically, Gaussian models contain modules parameterizing the important processes affecting dilution. Such modules may deal with dispersion coefficients, plume rise, wind shear and plume reflection and surface characteristics.

The dispersion coefficients σ_y and σ_z describe the spatial distribution of the dispersion material as a function of stability and distance downwind. There are several sources in the literature of empirically derived values of σ_y and σ_z, eg,Turner (1973), Carpenter (1971), Misra et al (1980). The most appropriate σ_y and σ_z values would be those measured at the site being modelled. This is possible for the Nanticoke site by using the values of Misra et al (1980). These values are also recommended for stations where lake influences are present. However, for power plants where lake effects are not important the values prescribed by Carpenter (1971) are recommended.

Plume rise is represented in Equation 1.0 by H. H is primarily a function of the plume's exit temperature and velocity, the former often being the dominant mechanism for power plant plumes. A plume rise model tuned with data collected at Nanticoke TGS has been developed, Edwards (1983), and is recommended for use with the trace element dispersion model selected.

Wind shear modules recognize the condition that wind speeds are usually greater aloft than those observed at or near ground level and that wind direction often changes significantly with height. Again the use of site specific data is desirable; however, when not available, an exponential wind speed profile and an Ekman spiral model are often used instead. The wind shear model 'CRSTER' is recommended.

Most models contain reflection terms R(Hm) as indicated in Equation 1.0. These terms account for reflection of the plume at the ground and at a mixing height aloft. Usually, empirically derived mixing height algorithms based on data such as those of Portelli (1977) are used.

Often the effects of mesoscale features such as lake/land breezes are treated implicitly in Gaussian models by the inclusion of a surface characteristic module. This module also is important to the dry deposition module discussed in the Part I report. Typically, representative surface roughness lengths for annular segments of the surrounding terrain are input, Sehmel and Hodgson (1978). The CEA/ Battelle 'CLIDE' model has a state-of-the-art treatment of surface characteristics.

The above discussion has covered those processes which affect plume dilution. In addition to those modules it is necessary to include modules which deplete the plume. The important depletion processes are dry and wet deposition. State-of-the-science descriptions of these processes have been presented in the Phase I report, Kalvins (1983). It is recommended that the modules offered by the CEA/ Battelle 'CLIDE' model be used to represent these processes.

To facilitate the calculation of plume depletion using the modular approach recommended here, the Gaussian transport and dispersion model should be configured such that depletion is determined for predefined sectors based on the surface characteristics surrounding the generating station.

Given the time scales of interest (ie, seasonal and longer) and the available input data, a group of Gaussian models, known as climatological models, is prescribed. A Gaussian climatological transport and dispersion model is driven by seasonal or longer time average frequency distributions of meteorological parameters such as wind speed, wind direction, stability and precipitation. There are many Gaussian climatological models available in the literature. Some examples are listed in Table I.

TABLE I

Model	Organization
AQSTM	Illinois Environmental Protection Agency
AIM	Oak Ridge National Laboratory
CDM/CDMQC	US Environmental Protection Agency
CLIDE	Droppo, Allwind and Davis, 1982
CRSTER	US Environmental Protection Agency
GEM	Science Applications, Inc
ISC/ISCST	H.E. Cramer Company, Inc
MESOPUFF	Environmental Research and Technology Inc
MPTER	US Environmental Protection Agency
MSDM	Lawrence Livermore Laboratory
MULTIMAX	Shell Development Company
PAL	US Environmental Protection Agency
PHOENIX	Hobbs, Eltgroth, Hegg, Radke, 1983
PTDIS	US Environmental Protection Agency
PTAMX	US Environmental Protection Agency
PTMTP	US Environmental Protection Agency
RAM	US Environmental Protection Agency

SCIM	GEOMET, Inc
TCM	Texas Air Control Board
TEM	Texas Air Control Board
VALLEY	US Environmental Protection Agency

4.0 MODEL SELECTION CRITERIA

The information presented in the trace inorganic element reports, Part I and Part II may be synthesized to yield a proposed set of criteria for selecting a trace element deposition model for use by Ontario Hydro. The selection criteria developed are as follows:

- A Gaussian climatological model suitable for the transport and dispersion of gaseous and particulate trace element emissions, containing state-of-the-art modules (as prescribed in this report) for plume rise, wind shear, reflection, dispersion coefficients, gravitational sedimentation, wet and dry deposition, and particle size distribution.

- The modelling region of interest should be within a radius of 25 km of the source.

- The model should be capable of computing seasonal or longer time average.

- The model should be tunable for surface characteristics surrounding the Nanticoke, Lakeview, Lambton, Atikokan and Thunder Bay power plants.

- The model must be implementable on an Ontario Hydro computer.

- The model should use a practical amount of computer time and the software should be user friendly.

5.0 CONCLUSIONS AND RECOMMENDATIONS

It is apparent from the two survey reports that significant knowledge gaps exist which prevent the quantitative determination of trace element deposition. For example, deposition velocities and scavenging coefficients are not known for most trace elements. Similarly, little empirical or theoretical information exists on in-plume transformations of trace element emissions. However, it is possible with what is currently known to assemble a 'state-of-the-art' model with which estimates of trace element deposition may be made. This report presents criteria for selecting such a model. Subsequent phase of the investigation of trace element deposition will involve applying the selection criteria to the models listed in Table I. The final result will most likely be a hybrid model composed of the best modules from the models in Table I.

It is likely that Ontario Hydro will require more information on its trace element emissions for each of the power plants of interest (ie, Nanticoke, Lakeview, Atikokan, Lambton and Thunder Bay TGS) and will require more sampling of trace element concentrations at these plants.

As part of this work the CEA/Battelle Pacific Northwest Labs Phase I and Phase II reports were reviewed. This work represents a comprehensive review of the current knowledge in this field. The report presented a trace element deposition model and modelling results for Nanticoke TGS. The report concluded from the modelling that effects of trace element emissions at Nanticoke were not significant. Insufficient detail on the modelling was provided in the Battelle report to critically assess this conclusion. Phase III of the trace element work will involve obtaining more detail on the Battelle model.

Apparently the work on trace element emissions will continue with funding from EPRI/Battelle. Ontario Hydro should continue to follow the progress of this work.

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